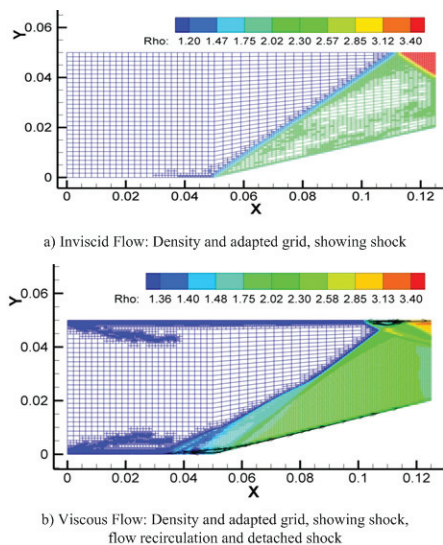


Adaptive Finite Element Methods for Combustion Modeling

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To facilitate predictive combustion modeling, in particular simulation of internal combustion engines, we are developing *hp*-adaptive finite element methods (FEM) and software that provide a high degree of accuracy and solution robustness. We have developed an FEM projection method, a predictor-corrector scheme (PCS), that has excellent capability over all flow regimes, from incompressible to supersonic flow. The system is applicable to Newtonian and non-Newtonian fluids, multi-species flow, and multi-phase (with spray/injection modeling). These algorithms are capable of representing the physics within an engine. We continue to provide software that many use directly for engine simulation or that they may alter with various models such as sophisticated chemical kinetics, different turbulent closure methods, or other fuel injection methods. Currently the software (KIVA) is in worldwide use for research. We are working to deliver a more predictive capability that when put to use by researchers and corporations should help in our understanding of internal combustion engines, providing for greater efficiency.

Fig. 1. Density contours and adapted grid for 2D Mach 2.22 through a 15° compression ramp: a) Inviscid flow, b) Viscous flow



To facilitate predictive combustion modeling, in particular simulation of internal combustion engines, we are developing methods that provide a high degree of accuracy and robustness of solution. We also continue to improve the physics modeling methods, with addition of appropriate turbulence closure schemes. We have developed a projection method, a predictor-corrector scheme (PCS) that has excellent capability over all flow regimes, from incompressible to supersonic flow. The system is applicable to Newtonian and non-

Newtonian fluids, multi-species flow and multi-phase (with spray/injection modeling). This PCS algorithm can also be used for porous media, solidification, or incompressible solid mechanics modeling with use of appropriate constitutive models.

This PCS method, combined with higher-order polynomial approximation for model-dependent physical variables (*p*-adaptive) along with grid enrichment (locally higher grid resolution-*h*-adaptive) and overset grids for actuated and immersed moving parts, will provide for a high order of accuracy and robust solutions in the next generation of KIVA, particularly on complex domains.

We continue to provide software that others may use directly or that they may alter with various component models such as sophisticated chemical kinetics, different turbulent closure methods, or other fuel injection methods. Our current users are worldwide, from individuals and small research

institutions to large corporations. We expect to be able to deliver a more predictive and robust modeling capability that, when put to use by these users, should help in our understanding of internal combustion engines. With that understanding, even greater efficiency should result. We expect sufficient changes in efficiency that we anticipate saving 4 million barrels of fuel per day in the US transportation fleet when this work is combined with other research and innovations in the field. Along with reduced fuel use, greater model predictability will help to reduce dangerous combustion products.

Proceeding with the idea in mind that it is better to have algorithms that are more accurate at a given resolution and provide for higher resolution and accuracy only where and when required, we recently began researching the use of adaptive finite element methods (FEM) [1]. Our construction is a Galerkin-type FEM that utilizes conservative momentum and energy transport. The projection scheme uses precise Petrov-Galerkin stabilization and pressure stabilization.

Projection methods are enjoying great popularity in the finite element community for good reason. These methods, combined with higher-order polynomial approximation for model-dependent physical variables (*p*-adaptive) along with grid enrichment (locally higher grid resolution-*h*-adaptive) and overset grids for actuated and immersed moving parts, are providing for highly accurate and robust solutions in the next generation of KIVA, particularly on complex domains. We have been developing this PCS algorithm for KIVA from our *h*-adaptive and *hp*-adaptive FEM research to create a new KIVA combustion code [2-5].

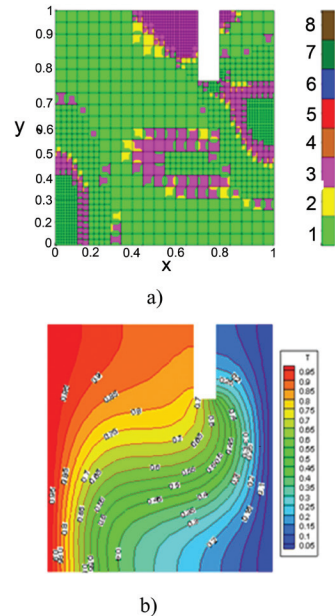


Fig. 2. Partially divided differentially heated enclosure; a) final hp -adaptive mesh, b) isotherms.

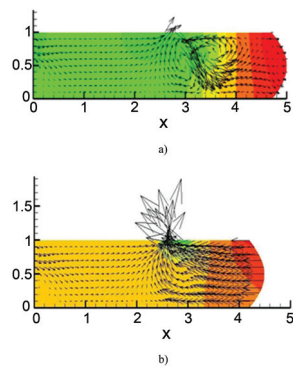


Fig. 3. Immersed moving piston for PCS FEM system; a) and b) showing displacement, velocity vectors (color represents isobars variation).

The immersed actuated parts in the engine are represented by an unstructured overset grid system where local adjustments to the fluid grid occur only when the actuated parts cross the boundary of a fluid element, a robust scheme that works for complex domains. The method maintains second-order spatial accuracy, and is a form of Arbitrary Lagrangian Eulerian (ALE) method, where the fluid grid moves only locally to accommodate a moving overset grid representing the part, such as a valve or piston. Once the part leaves an element, or when the part is outside an element, the element returns to its original shape.

Figure 1 shows the h -adaptive solution for both inviscid and viscous Mach 2.22 supersonic flow through a 2D compressor. The inviscid solutions are in exact agreement with the analytical solution, with the viscous solution agreeing with similar solutions [6]. The flow in Fig. 1b includes the viscous terms, and the algorithm is capable of capturing the small zones of recirculation in front to the main shock.

Verification results shown in Fig. 2 are using a PCS fractional-step algorithm [1,4], natural convection in a partially divided enclosure. The left and right walls are maintained at hot and cold temperatures respectively. Figure 2a shows the final hp -adaptive mesh where the initial coarse mesh consisted of 388 quadrilateral elements with 435 nodes; the final mesh consists of 1,261 elements and 4,714 degrees of freedom.

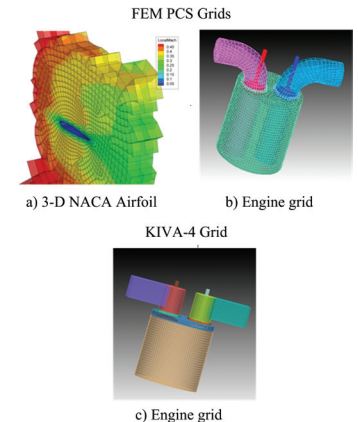
In Fig. 3, a 2D piston is shown at two different times during the cycle. The solution is performed for incompressible flow to facilitate development and validation. Error for this formulation against a known solution (a benchmark) is one percent or less depending on resolution; the method shows second-order spatial convergence.

The use of Cubit [http://cubit.sandia.gov/] for engine grid generation is being investigated. Once the grid is implemented in a script language, the grid generation process is automatic. The scripts are often easily altered for various engine domains and grid refinements. This work supports our effort to produce unstructured hexahedral engine grids that are essentially automatic. The file converter from Cubit output has been developed for both KIVA-4mpi and the new FEM formulation. Because the FEM grid is designed for use with the overset grid scheme

discussed previously, it is much easier to produce a quality grid (almost automatically) than it is for the current KIVA-4 using an unstructured grid and the old actuated parts system. The Cubit grids for an airfoil validation problem and for an internal combustion engine are shown in Fig. 4.

Our work continues by: 1) extending the moving parts algorithm to 3D, 2) adding KIVA's injection/spray and chemistry packages to the FEM version, and 3) implementing the method for solving engine simulations using multi-processors (that is, in solutions run in parallel manner).

Fig. 4. Cubit grid generation for FEM KIVA and for KIVA-4 using all hexahedral elements; a) NACA-0012 local mach values from PCS algorithm, b) grid for PCS algorithm, c) grid for KIVA-4.



- [1] Carrington, D.B., "A Fractional Step hp -adaptive Finite Element Method for Turbulent Reactive Flow," LANL Technical Report LA-UR-11-00466 (2011).
- [2] Carrington, D. B. et al., *Comput Model Eng Sci* **61**, 23 (2010).
- [3] Wang, X. et al., *Comput Therm Sci* **1**, 121 (2009).
- [4] Carrington, D.B., "A Characteristic-based Split hp -adaptive Finite Element Method for Combustion Modeling in KIVA-hpFE," LANL Technical Report LA-UR-09-06527 (2009).
- [5] Wang, X. and D. W. Pepper, *J Thermophys Heat Tran* **21**, 190 (2007).
- [6] Breuckner, F.P. and Heinrich, J.C., *Int. J. Numer. Meth. Fluids* **32**, 255 (1991).

Funding Acknowledgments

DOE, Office of Energy Efficiency and Renewable Energy, Vehicle Technology Program